

Phase Separation in Mixtures of Repulsive Fermi Gases Driven by Mass Difference

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We show that phase separation must occur in a mixture of fermions with repulsive interaction if their mass difference is sufficiently large. This phenomenon is highly dimension-dependent. Consequently, the density profiles of phase separated 3d mixtures are very different from those in 1d. Noting that the ferromagnetic transition of a spin-1/2 repulsive Fermi gas is the equal mass limit of the phase separation in mixtures, we show from the Bethe Ansatz solution that a ferromagnetic transition will take place in the scattering states when the repulsive interaction passes through resonance and becomes attractive.

In the last few years, there have been considerable interests in strongly repulsive Fermi gases. Many of these studies were stimulated by the report of evidence of ferromagnetism in the Fermi gas of ${}^6\text{Li}$ [1]. The possibility of itinerant ferromagnetism was first proposed by Stoner for electron gas[2]. The idea is that if Coulomb repulsion increases faster than kinetic energy as a function of increasing density as indicated by Hartree-Fock estimates, the system will turn ferromagnetic and form ferromagnetic domains at sufficiently high densities. However, Hartree-Fock approximation overestimates repulsion energy. So far, itinerant ferromagnetism has not been found in metals.

Itinerant ferromagnetism had also been predicted for strongly repulsive Fermi gas based on perturbative and mean field calculations[3, 4] prior to the MIT experiment [1]. However, such approaches are known to be unreliable in strongly interacting regime. In fact, no ferromagnetic domain were observed in ref.[1], and newer experiments have established that the repulsive Fermi gas of ${}^6\text{Li}$ is non-magnetic [5]. This shows that within the range of interaction studied experimentally, the repulsion in Fermi gases does not dominate over the kinetic energy as mean field calculations show. Yet Stoner's idea should work. It should also be applicable to systems such as binary mixtures of Fermi gases, (referred to as Fermi-Fermi mixture for short). In that case, the analog of ferromagnetic transition of spin-1/2 Fermi gas is phase separation of the two fermion species.

Phase separation of Fermi-Fermi mixtures has been studied in ref.[6] using mean field approximation and perturbation methods. It is found that a ${}^6\text{Li}$ - ${}^{40}\text{K}$ mixture will phase separate in the strongly interacting regime. Since the same mean field theory predicts a ferromagnetic transition in a spin-1/2 Fermi gas in the strongly interacting regime[4] which is not observed[5], it raises the questions about whether increasing repulsion can in fact cause a Fermi-Fermi mixture to phase separate as mean field theory predicts.

In this paper, we would like to point out that phase separation in a Fermi-Fermi mixture can always be induced by increasing the mass ratio of the two fermion

species, but not necessarily by increasing repulsion. The reason is that the kinetic energy cost for phase separation can always be reduced to zero by increasing the mass ratio, thereby falling below the repulsion energy, rendering the Stoner argument valid. On the other hand, since the density regime for strong interaction is dimension dependent, the phenomena of phase diagram changes significantly with dimensionality. Since the ferromagnetic transition in spin-1/2 systems (which leads to formation of domains) is the equal mass limit of the phase separation of Fermi mixtures, it is useful to unify these two phenomena with a global phase diagram as a function of mass ratio and interaction. In the 1d case, we shall also show from exact result that an “upper-branch” spin-1/2 Fermi gas will turn ferromagnetic as it passes through resonance to the side of attractive interaction.

(A). *A theorem on mass-difference driven phase separation:* The energy density \mathcal{E}_{hm} of the ground state of a homogenous mixture of heavy and light fermions with masses (m_L , m_H) and densities (n_L , n_H) is

$$\mathcal{E}_{hm} = \mathcal{E}_L + \mathcal{E}_H + \mathcal{E}_L G\left(\frac{m_L}{m_H}, n_L^{1/d} a, \frac{n_H}{n_L}\right), \quad (1)$$

where $\mathcal{E}_{L(H)}(n_{L(H)}) = A_d n_{L(H)}^{(2+d)/d} / m_{L(H)}$ is the energy density of the ideal gas of the light (heavy) fermions, d is the dimensionality, and A_d is a constant. The last term $U = \mathcal{E}_L G$ is the interaction energy in units of \mathcal{E}_L , and G is a dimensionless function of the variables displayed. “ a ” is the length scale associated with the interaction. In 3d, a is the s-wave scattering length a_s in the pseudo-potential

$$\hat{U} = \frac{2\pi a_s}{m} \sum_{i>j} \delta(\mathbf{r}_{ij}) \left(\frac{\partial}{\partial \mathbf{r}_{ij}} r_{ij} \right), \quad \frac{1}{m} = \frac{1}{m_L} + \frac{1}{m_H}. \quad (2)$$

We set $\hbar = 1$ in this paper. By applying harmonic confinement along the axial (with frequency ω_z) or the transverse (ω_\perp) direction, the system can be reduced to a quasi 2d or a quasi 1d system. For quasi 2d systems, a is related to the binding energy as $\epsilon_b = 1/(2\bar{m}a^2)$, where $\epsilon_b = \frac{B}{\pi} \omega_z e^{\sqrt{2\pi} a_z / a_s}$, $a_z = \sqrt{1/(\bar{m}\omega_z)}$ is the confinement length and $B \approx 0.915$ [7]. For quasi 1d sys-

tems, $a = -\frac{a_{\perp}}{2}(\frac{a_{\perp}}{a_s} - C)$ where $a_{\perp} = \sqrt{1/(\overline{m}\omega_{\perp})}$ and $C \approx 1.46$ [8]. In all dimensions, the energy satisfies the

adiabatic theorem, $\partial E_{hm}/\partial \zeta > 0$, where ζ are $-1/a$ [9], $\ln a$ [10] and a [11] respectively for 3d, 2d and 1d systems.

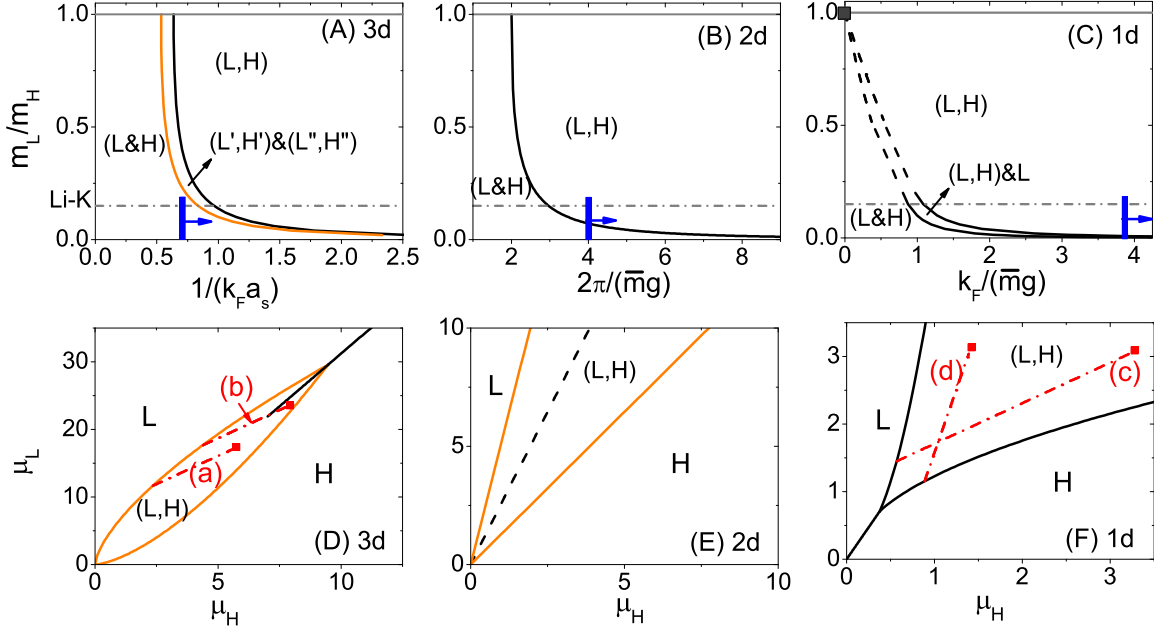


FIG. 1. Figure 1A, 1B, and 1C are the phase diagrams for a 3d, 2d, and 1d Fermi-Fermi mixture with $N_L = N_H$ in a volume V . $k_F = (6\pi^2 n)^{1/3}$ and πn respectively for 3d and 1d, with $n = N_L/V = N_H/V$. To the right of the vertical blue line, the mean-field interaction energy is less than half of total kinetic energy for a homogenous mixture (L,H), and the system is weakly interacting deeper in that region. The gray dashed-dot lines indicate the case of a Li-K mixture with $m_L/m_H = 6/40$. Figure 1D, 1E, and 1F are the phase diagrams of a 3d, 2d, and 1d Li-K mixture in chemical potential plane for weak interactions. μ_H, μ_L are scaled by $(\overline{m}^d g^2)^{1/(2-d)}$ in 3d and 1d, and $1/\overline{m}$ in 2d. The red dashed-dotted lines in 1D and 1F represent trajectories for the density profiles of a trapped system, corresponding to (a-d) in Fig.2, with the squares denoting the chemical potentials at the trap center. From Figure 1A to 1F, the black (orange) solid lines represent the 1st (2nd)-order boundaries with (without) density discontinuity. In Figure 1B, the boundary is given by the function $g_c(m_L, m_H) = 2\pi/\sqrt{m_L m_H}$. In 1E, the two solid orange lines are the boundaries for interaction $g < g_c$, with two slopes $(g/g_c)\sqrt{m_H/m_L}$ and $(g_c/g)\sqrt{m_H/m_L}$ respectively. When $g \geq g_c$, the two boundaries merge into one (shown by dashed line) with slope $\sqrt{m_H/m_L}$.

To find the condition for phase separation, we consider a system with N_L and N_H fermions in a volume V . Let us define

$$m_L/m_H \equiv x, \quad N_H/N_L \equiv \gamma, \quad (3)$$

the total energy of the homogenous mixture is

$$E_{hm} = V\mathcal{E}_L(n_L)(1 + \gamma^\alpha x + G), \quad \alpha = 1 + 2/d. \quad (4)$$

Next, we consider the fully phase separated state. Let V_H and V_L be the volumes of the heavy and light fermions, $V_H + V_L = V$. The ratio V_H/V_L is determined by equating the pressure P of these two separated gases. Since the pressure of an ideal gas is proportional to its energy density, $P = 2\mathcal{E}/d$, we have $\mathcal{E}_L(n'_L) = \mathcal{E}_H(n'_H)$, where $n'_{H(L)} = N_{H(L)}/V_{H(L)}$. This gives $V_H/V_L = \gamma x^{1/\alpha}$.

The total energy of the phase separated state is $E_{PS} = V_H\mathcal{E}_H(n'_H) + V_L\mathcal{E}_L(n'_L) = V\mathcal{E}_L(n_L)(V/V_L)^{(2+d)/d}$, or

$$E_{PS} = V\mathcal{E}(n_L) \left(1 + \gamma x^{1/\alpha}\right)^\alpha. \quad (5)$$

The phase separated state will have lower energy if $E_{hm} - E_{PS} > 0$, or

$$I(x) = G(x) - \left[(1 + \gamma x^{1/\alpha})^\alpha - 1 - \gamma^\alpha x\right] > 0. \quad (6)$$

When the mass ratio is sufficiently small such that $\gamma^{1/\alpha} x \ll 1$, hence $x^\alpha < x$, Eq.(6) becomes

$$I(x) = G(0) - \alpha\gamma x^{1/\alpha} + O(x, x^{2/\alpha}) > 0, \quad (7)$$

where $G(0) > 0$ is the repulsive interaction energy in the limit when $m_H \rightarrow \infty$ [12]. Eq.(7) can always be satisfied

for sufficiently small x , thus proving that phase separation must occur for sufficiently large mass difference.

Corollary: Because of the adiabatic theorem, if a mixture with mass ratio m_L/m_H phase separates at a given interaction ζ , it will continue to phase separate at stronger interactions, i.e. at a larger ζ .

(B). *Phase diagram:* To be concrete, we shall consider the phase diagram for weak repulsion. In this case, the interaction energy U in Eq.(2) is much less than the kinetic energy, and is accurately described by the mean field form $U = gn_L n_H$, where $g = \frac{2\pi a_s}{m}$ in $3d$, $\frac{2\sqrt{\pi}}{m} \frac{a_s}{a_z}$ in quasi $2d$, and $\frac{2}{m} \frac{a_s}{a_{\perp}^2}$ in quasi $1d$. The energy density \mathcal{E}_{hm} , chemical potential (μ_L, μ_H) for light and heavy particles, and the pressure of the homogenous mixture are

$$\mathcal{E}_{hm}(n_L, n_H) = \mathcal{E}_L(n_L) + \mathcal{E}_H(n_H) + gn_L n_H, \quad (8)$$

$$\mu_{L(H)}(n_L, n_H) = \frac{\partial \mathcal{E}_{L(H)}(n_{L(H)})}{\partial n_{L(H)}} + gn_{H(L)}, \quad (9)$$

$$P(n_L, n_H) = \mu_L n_L + \mu_H n_H - \mathcal{E}(n_L, n_H). \quad (10)$$

For a system with N_L light fermions and N_H heavy fermions in a volume V , the possible configurations are: (a) fully phase separated state (PS), denoted as $(L\&H)$; (b) coexistence of a homogenous mixture and a single phase, denoted as $(L, H)\&L$ or $(L, H)\&H$; (c) coexistence of two homogeneous mixtures with different densities (n'_L, n'_H) and (n''_L, n''_H) , denoted as $(L', H')\&(L'', H'')$; and (d) a single homogenous mixture (L, H) . To determine the presence of these phases, it is sufficient to consider the general situation $(L', H')\&(L'', H'')$, since it covers all other cases. For example, the state $(L\&H)$ corresponds to $n'_H = n''_L = 0$. The state $(L, H)\&L$ corresponds to $n'_H = 0$, and the state (L, H) corresponds to $n'_L = n''_H = 0$.

Let us denote the particle numbers in the two coexistent homogenous mixtures as (N'_L, N'_H) and (N''_L, N''_H) , and their volumes as V' and V'' , where $N'_L + N''_L = N_L$, $N'_H + N''_H = N_H$; and $V' + V'' = V$. Minimizing the total energy with respect to N'_L, N'_H and V' will determine the type of configuration ((a) to (d)) for given interaction, from which one can construct the phase diagram. In the cases of (b) and (c), the minimization procedure leads to the Gibbs phase rules, i.e. two coexisting phases have the same pressure and the same chemical potential for the same atomic species.

The phase diagram of a $3d$ mixture as a function of chemical potential and interaction has been studied in ref.[6]. Here, we examine the phase diagram in different dimensions, focusing on the effect of mass ratio. Figure 1A, 1B, and 1C show the phase diagrams for a $3d$, $2d$, and $1d$ mixture with $N_L = N_H$ in a volume V . In all cases, the system is fully phase separated $(L\&H)$ for sufficiently small mass ratio m_L/m_H . For both $1d$ and $3d$, there is a range of mass ratio (for given interaction) in which the system consists of two different phases in equilibrium,

$((L, H)\&L$ for $1d$ and $(L', H')\&(L'', H'')$ for $3d$). This feature is absent in $2d$ [13].

Note that the phase boundaries in Figure 1A to 1C are derived from the weak coupling form of the interaction, they are therefore inaccurate in the strongly interacting region. However, the corollary in section (A) guarantees that the system will phase separate in the strongly interacting region over a range of mass ratio wider than that in the weakly interacting region.

(C) *Ferromagnetic transition of $1d$ spin-1/2 Fermi gas at resonance:* The phase diagram for $1d$ Fermi-Fermi mixture is not only constraint by the results in the weakly interacting regime, but also by the exact Bethe Ansatz solution along the line $m_L/m_H = 1$ [14], which is a spin-1/2 repulsive Fermi gas with interaction $g \sum_{i>j} \delta(x_i - x_j)$, where $g = -(\bar{m}a)^{-1}$. Because of the integrability of this system, there are two classes of eigenstates: one where all quasi-momenta are real, i.e., all particles are in scattering states, (denoted as class (i)), and one that contains at least one pair complex conjugate quasi-momenta, i.e. with at least one fermion bound pair, (denoted as class (ii)). Repulsive Fermi gas is in class (i). It is stable without decay into class (ii)[15]. System in class (i) will be referred to as in the ‘‘upper branch’’.

Experimentally, one can tune the interaction from the repulsive regime ($-1/g < 0$) to the strongly repulsive regime near resonance ($-1/g = 0^-$), and then to strongly attractive regime ($-1/g = 0^+$). The ground state of a repulsive ($-1/g < 0$) spin-1/2 Fermi gas with equal spin population is a spin-singlet according to the Lieb-Mattis theorem[16]. Its energy is a monotonically increasing function of $-1/g$ according to the adiabatic theorem. At resonance, $-1/g = 0$, the spatial wavefunction of the ground state is identical to that of a fully spin polarized Fermi gas up to a sign (which changes in various regions in configuration space). As a result, its energy $E(0)$ is given by that of a fully spin polarized state with huge spin degeneracy[14] – all spin configurations including the spin configurations (a) to (c) mentioned above are degenerate, with H and L now labeling the two spin species. This means that the two phase boundaries in Fig.1C will converge to the equal mass point $m_L/m_H = 1$ at resonance. Crossing the resonance to the attractive side, $-1/g > 0$, the energies of all spin states continue to increase, hence $E(-1/g > 0) > E(0)$; except for the largest spin state which remains at $E(0)$ regardless of interaction. The system will therefore make transition to this maximum spin state. In the presence of a small magnetic field with a weak field gradient that destroys spin conservations, the spin in the ground state will align along the field direction.

The equal mass line in Fig.1C shows that the system will not phase separate (or turn ferromagnetic) even when repulsion is made the strongest (i.e. at resonance). Similar situation occurs in $3d$. There, experiments show that the spin-1/2 Fermi gas is not ferromagnetic (i.e.

no phase separation) at all strongly interacting regime examined[5]. Instead, by increasing the mass difference, the repulsive mixture can definitely phase separate in any dimension, as guaranteed by the theorem in Section (A).

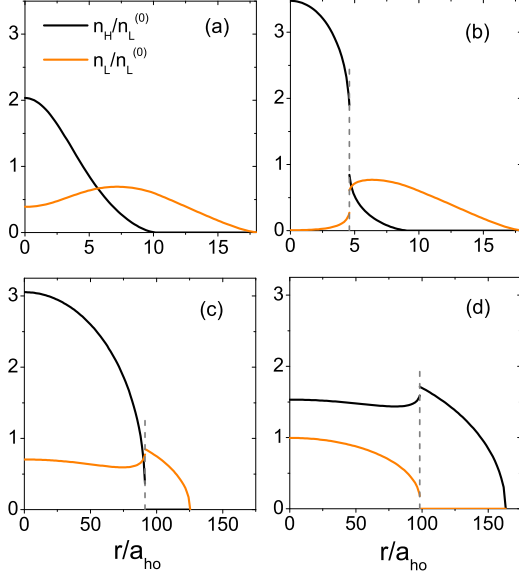


FIG. 2. Density profiles of a trapped Li(Light)-K(Heavy) mixture in 3d((a) and (b)) and 1d((c) and (d)), corresponding to the trajectories (a) to (d) in Fig.1D and 1F. The densities (n_H, n_L) have been normalized by $n_L^{(0)}$, the density of light atoms(Li) at the trap center for non-interacting system in the same setup. The position r is scaled by $a_{ho} = \sqrt{1/(m_L \omega_L)}$, the confinement length of light atoms. (a) and (b) are with the same particle numbers $(N_H, N_L) = (10^5)(1.47, 6.9)$ and the same trapping frequency ratio $\omega_H/\omega_L = 0.3$, but with different interaction strengths $a/a_{ho} = 0.055(a), 0.065(b)$. (c) and (d) are with the same $(N_H, N_L) = (10^4)(1.45, 0.51)$ and the same interaction $-a_{ho}/a = 15\pi$, but with different $\omega_H/\omega_L = 0.5(c), 0.2(d)$.

(D) *The density profile in a trap:* Phase separation can be easily identified in the density profile of a trapped gas, which can deduced from the phase diagram in the chemical potential $\mu_L - \mu_H$ plane. To illustrate the possible classes of phenomena, we again consider weak interactions.

Given μ_L and μ_H , three phases are allowed: the single component Fermi gas (L), (H), and the homogenous mixture (L, H). To express the pressure of a homogenous mixture P_{hm} as a function of μ_L, μ_H , we invert Eq.(9) to obtain n_L and n_H as a function of μ_L and μ_H , and then substitute them into Eq.(10). The pressure of (L) or (H) is $P_{L(H)}(\mu_L, \mu_H) = B_d m_{L(H)}^{d/2} \mu_{L(H)}^{1+d/2}$, where B_d is a constant. The phase boundary for the full phase separation is $P_L(\mu_L) = P_H(\mu_H)$, or

$$\mu_H/\mu_L = \beta, \quad \beta = (m_L/m_H)^{d/(d+2)}. \quad (11)$$

The phase boundary between the mixture (L, H) and L (or (H)) is obtained by equating $P_{hm}(\mu_L, \mu_H) = P_{L(H)}(\mu_{L(H)})$. The phase boundaries for the 3d, 2d, and 1d mixtures are shown in Figure 1D, 1E, and 1F respectively. Within the region of homogenous mixture, the inversion of Eq.(9) may yield several solutions of densities (say, (n'_L, n'_H) , (n''_L, n''_H)) for given chemical potentials (μ_L, μ_H) , which in general have different pressures. The thermodynamic state is given by one with highest pressure. In the 3d case, the homogeneous mixture is contained within the “bubble” in Figure 1D. Within this region, the thermodynamic state is unique except on the line that is an extension of the boundary Eq.(11) where two states (with densities (n'_L, n'_H) , (n''_L, n''_H)) have identical chemical potential and pressure. The difference in density across the boundary can be obtained by noting that the thermodynamic relations (Eq.(8) to (10)) of the mixture is invariant under the transformation

$$n_L \rightarrow n'_L = \beta n_H, \quad n_H \rightarrow n'_H = \beta^{-1} n_L, \quad (12)$$

The density discontinuities across this line are then $\Delta n_L = \beta n_H - n_L$, $\Delta n_H = \beta^{-1} n_L - n_H$, which implies

$$\Delta n_L / \Delta n_H = -\beta. \quad (13)$$

In Fig.2a to 2d, we show the density profiles of the 3d and 1d mixtures in a trap constructed by applying local density approximation (LDA) to the equation of state $n_{L(H)}(\mathbf{r}) = n_{L(H)}(\mu_L - V_L(\mathbf{r}), \mu_H - V_H(\mathbf{r}))$, where $V_L(\mathbf{r})$ and $V_H(\mathbf{r})$ are the potentials experienced by the light and heavy particles. Moving from the center of the trap to the surface of the cloud corresponds to following the trajectories indicated in Fig.1D and 1F. Fig.2a and 2b show the density profiles of a 3d mixture at different interaction strengths. The discontinuities of the densities follow Eq.(13). Fig.2c and 2d show a 1d mixture under different trapping potentials.

Two features of the density profiles should be emphasized. Firstly, the density profiles of a 3d mixture differ significantly from that of the 1d mixture, (see Fig.1D and 1F). Phase separation takes place in the outer part of the atom cloud in 1d but in the inner part in 3d. This is because the strongly interacting regime occurs in the low (high) density region in 1d (3d). Secondly, in Fig. 2a-2d, we note that $n_{L(H)}$ can increase with r . This is different from the single component case, where $dn/dr < 0$, due to the fact that $dn/d\mu > 0$ as demanded by thermodynamic stability. In the mixture case, stability against density fluctuation requires $\text{Det}(M) > 0$, where $M_{ij} = \partial \mu_i / \partial n_j$, and $i, j = L$ and H . We then have $dn_i/dr = (M^{-1})_{ij} dn_j/dr$, where $M^{-1} = \text{Det}^{-1}(M) \begin{pmatrix} A_H & -g \\ -g & A_L \end{pmatrix}$, $A_{L(H)} = \frac{\partial \mu_{L(H)}}{\partial n_{L(H)}} > 0$. That $dn_{L(H)}/dr$ can be positive or negative is because it is made up of two terms. If $dn_L/dr > 0$, it is easily shown from stability condition ($A_L A_H > g^2$) that $dn_H/dr < 0$.

Thus one can have at most one species with a positive density derivative.

Finally, we point out that the mass-difference mechanism for phase separation discussed in Section (A) will also be effective for mixtures with more atomic species; and the original Stoner idea will be illustrated most readily in the large mass difference limit. The features mentioned in this section, and the ferromagnetic transition of an upper branch spin-1/2 Fermi gas as implied by Bethe Ansatz should all be experimentally observable.

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